

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 8.80e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.59e-01

Confidence level: 3.82e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Triforine</div> <div>Measured: 2.89e-08</div> <div>Predicted: 2.34e-07</div>	<div>Image not found</div> <div>Formetanate hydrochloride</div> <div>Measured: 1.50e-07</div> <div>Predicted: 1.86e-07</div>	<div>Image not found</div> <div>Bensulfuron-methyl</div> <div>Measured: 5.16e-05</div> <div>Predicted: 6.38e-13</div>
<div>Image not found</div> <div>Fenpicionil</div> <div>Measured: 7.50e-09</div> <div>Predicted: 3.72e-07</div>	<div>Image not found</div> <div>Tetralin</div> <div>Measured: 1.00e-05</div> <div>Predicted: 4.25e-01</div>	